3-Ethyl-3-hydroxymethyl oxetane

Other names: 3-ethyloxetane-3-methanol
Inchi: InChI=1S/C6H12O2/c1-2-6(3-7)4-8-5-6/h7H,2-5H2,1H3
InchiKey: UNMJLQGKEDTEKJ-UHFFFAOYSA-N
Formula: C6H12O2
SMILES: CCC1(CO)COC1
Mol. weight [g/mol]: 116.16
CAS: 3047-32-3

Physical Properties

Property code	Value	Unit	Source
gf	-180.14	kJ/mol	Joback Method
hf	-369.52	kJ/mol	Joback Method
hfus	13.10	kJ/mol	Joback Method
hvap	49.07	kJ/mol	Joback Method
log10ws	-0.34		Crippen Method
logp	0.405		Crippen Method
mcvol	96.280	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
tb	467.06	K	Joback Method
tc	655.25	K	Joback Method
tf	283.09	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.48	J/mol×K	467.06	Joback Method
cpg	230.39	J/mol×K	498.42	Joback Method
cpg	240.54	J/mol×K	529.79	Joback Method
cpg	250.01	J/mol×K	561.15	Joback Method
cpg	258.89	J/mol×K	592.52	Joback Method
cpg	267.24	J/mol×K	623.88	Joback Method
cpg	275.16	J/mol×K	655.25	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3047323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume